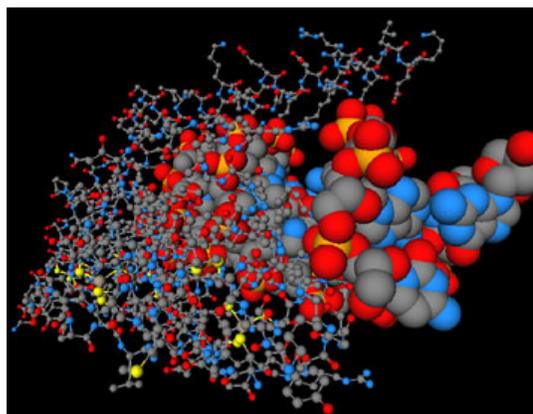


Ecce Version 3.2

The Extensible Computational Chemistry Environment (Ecce) provides a sophisticated graphical user interface, scientific visualization tools, and the underlying data management framework enabling scientists to efficiently set up calculations and store, retrieve, and analyze the rapidly growing volumes of data produced by computational chemistry studies.

Ecce Version 3.2, released on May 10, 2004, provides users with enhanced features supporting molecular dynamics calculations, including a force field editor and topology viewer. A new tool has been added to Ecce's arsenal—the DNA toolkit—which creates model segments of double-stranded DNA from arbitrary combinations of the four base pairs that are fundamental to all life. The new repertoire of capabilities in Ecce increases the accessibility of powerful modeling tools that can be employed to understand critical processes, such as DNA-protein interactions and catalytic reactions.



Ecce enables investigation of processes such as DNA-protein interactions and catalytic reactions.

With nearly 5 new user agreements each week, Ecce has been distributed to more than 500 sites worldwide, from Europe to South America and Asia. Available on multiple platforms, Ecce operates on most scientific computer systems, including Linux-based, Sun, and SGI workstations. Widely used by computational chemists and experimentalists, Ecce is also increasingly employed by educators to demonstrate basic molecular building and simulations.

Ecce was developed at the W.R. Wiley Environmental Molecular Sciences Laboratory. For information, see <http://ecce.emsl.pnl.gov>.

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